

# Local-Ansatz Approach with Momentum Dependent Variational Parameters to Correlated Electron Systems

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A new wavefunction which improves the Gutzwiller-type local ansatz method has been proposed to describe the correlated electron system. The ground-state energy, double occupation number, momentum distribution function, and quasiparticle weight have been calculated for the half-filled band Hubbard model in infinite dimensions. It is shown that the new wavefunction improves the local-ansatz approach (LA) proposed by Stollhoff and Fulde. Especially, calculated momentum distribution functions show a reasonable momentum dependence. The result qualitatively differs from those obtained by the LA and the Gutzwiller wavefunction. Furthermore, the present approach combined with the projection operator method CPA is shown to describe quantitatively the excitation spectra in the insulator regime as well as the critical Coulomb interactions for a gap formation in infinite dimensions.

**KEYWORDS:** variational method, electron correlations, Gutzwiller wavefunction, local ansatz, Hubbard model, excitation spectra, critical Coulomb interaction, infinite dimensions

## 1. Introduction

Variational method has been a useful tool to investigate the ground-state properties of correlated electrons from molecules to solids over half a century. In the method, a minimum basis set to describe correlated electrons is constructed by applying one-particle, two-particle, and higher-order particle operators onto the Hartree-Fock wavefunction, and their amplitudes are chosen to be best on the basis of the variational principle. Among various trial wavefunctions, the Gutzwiller wavefunction is one of the simplest and popular wavefunctions in solids. It was introduced by Gutzwiller to clarify the role of electron correlations in metallic ferromagnetism.<sup>1,2</sup> The idea is to reduce the amplitudes of doubly occupied states on the local orbitals in the Hartree-Fock wavefunction by making use of a projection operator  $\Pi_i(1 - gn_{i\uparrow}n_{i\downarrow})$ . Here  $n_{i\sigma}$  is the number operator for electrons on site  $i$  with spin  $\sigma$ . The variational parameter  $g$  is determined by the minimization of the ground-state energy. Later, it has been pointed out by Brinkman and Rice that the Gutzwiller wavefunction describes the metal-insulator transition.<sup>3</sup> Because the Gutzwiller method is a nonperturbative approach, it has extensively been applied to the strongly correlated electron systems such as the heavyfermions, high- $T_c$

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cuprates, and other transition metal oxides.<sup>4</sup>

Although the Gutzwiller ansatz approach (GA) captures the physics of electron correlations and is useful for correlation problems, it was not so easy to apply the method to realistic Hamiltonians. Stollhoff and Fulde proposed an alternative method called the local-ansatz approach (LA), which is simpler in treatment and applicable to realistic Hamiltonians.<sup>5,6</sup> The LA takes into account the excited states created by local two-particle operators such as  $\{O_i\} = \{\delta n_{i\uparrow}\delta n_{i\downarrow}\}$ , and determines their amplitudes variationally. Here  $\delta n_{i\sigma} = n_{i\sigma} - \langle n_{i\sigma} \rangle_0$ ,  $\langle n_{i\sigma} \rangle_0$  being the average electron number on site  $i$  with spin  $\sigma$  in the Hartree-Fock approximation. The LA has been applied to many systems such as molecules, polyacetylene, transition metals, semiconductors, and transition metal oxides.<sup>7</sup>

The LA is useful for understanding correlation effects in actual materials. The application however has been limited to the weakly correlated region because of the difficulty in evaluation of the higher-order terms in average quantities. In the weak interaction limit, the Hilbert space expanded by the local operators is, however, not enough to describe exactly the weakly correlated region; the LA does not reduce to the second-order perturbation theory in the weak correlation limit. The same difficulty also arises in the original Gutzwiller wavefunction even in infinite dimensions. In the present paper, we aim to solve these problems in the LA introducing a new wavefunction with momentum-dependent variational parameters, and demonstrate that the new approach much improves the LA in the weak and intermediate correlation regimes. In the following, we call the new approach the MLA (the LA with momentum dependent variational parameters).

We write down our wavefunction for the single-band Hubbard model in §2. The idea is to choose the best local basis set obtained from the two-particle excited states in the momentum representation by projecting out those states onto the local subspace and by controlling the amplitudes of the excited states in the momentum space. We calculate the ground-state energy within a single-site approximation. Using the variational principle, we determine the momentum-dependent variational parameters. The ground-state energy obtained from our wavefunction agrees with the result of the second-order perturbation theory in infinite dimensions in the weak interaction limit, and reduces to the correct atomic limit in the case of the half-filling.

In §3, we present the results of numerical calculations for the half-filled band Hubbard model in infinite dimensions to examine the validity of the new wavefunction. We calculate the correlation energy, the double occupation number, the momentum distribution function, and the quasiparticle weight as a function of the Coulomb interaction energy parameter. We verify that the present approach improves both the LA and the GA in the weak and intermediate Coulomb interaction regimes. In particular, we demonstrate that the momentum distribution calculated by our wavefunction (the MLA) shows a distinct momentum dependence, and

is qualitatively different from those obtained by the LA and GA leading to the constant values of the distribution function below and above the Fermi level. In §4, we present an example of applications to excitation problems. We have recently developed a self-consistent method<sup>8</sup> to calculate the excitation spectra from the retarded Green function by making use of the projection operator technique and the effective medium within the coherent potential approximation (CPA).<sup>9,10</sup> The method called the projection operator method CPA (PM-CPA)<sup>8</sup> is equivalent<sup>11,12</sup> to the many-body CPA,<sup>13</sup> the dynamical CPA,<sup>14,15</sup> and the dynamical mean field theory,<sup>16–19</sup> and treats the dynamics and the static correlations separately in the calculations. We calculate here the excitation spectra combining our variational method with the PM-CPA. We show that the calculated spectra in the insulator regime quantitatively agree with the results of the numerical renormalization group (NRG) calculations.<sup>20</sup> In the last section, we summarize our results and discuss future problems.

## 2. Local Approach with Momentum Dependent Variational Parameters

We consider in the present paper the single-band Hubbard model defined by

$$H = \sum_{i\sigma} (\epsilon_0 - \sigma h) n_{i\sigma} + \sum_{ij\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} . \quad (1)$$

Here  $\epsilon_0$  ( $h$ ) is the atomic level (magnetic field),  $t_{ij}$  is the transfer integral between sites  $i$  and  $j$ .  $U$  is the intra-atomic Coulomb energy parameter.  $a_{i\sigma}^\dagger$  ( $a_{i\sigma}$ ) denotes the creation (annihilation) operator for an electron on site  $i$  with spin  $\sigma$ , and  $n_{i\sigma} = a_{i\sigma}^\dagger a_{i\sigma}$  is the electron density operator on site  $i$  for spin  $\sigma$ .

In the Hartree-Fock approximation, we replace the many-body Hamiltonian (1) with an effective Hamiltonian for independent electrons,

$$H_0 = \sum_{ij\sigma} t_{ij\sigma} a_{i\sigma}^\dagger a_{j\sigma} - U \sum_i \langle n_{i\uparrow} \rangle_0 \langle n_{i\downarrow} \rangle_0 , \quad (2)$$

and approximate the ground-state wavefunction  $|\Psi\rangle$  with that of the Hartree-Fock Hamiltonian  $H_0$ , *i.e.*,  $|\phi_0\rangle$ . Here  $t_{ij\sigma} = (\epsilon_0 + U \langle n_{i-\sigma} \rangle_0 - \sigma h) \delta_{ij} + t_{ij}(1 - \delta_{ij})$ .  $\langle \sim \rangle_0$  denotes the Hartree-Fock average  $\langle \phi_0 | (\sim) | \phi_0 \rangle$ , and  $\langle n_{i\sigma} \rangle_0$  is the average electron number on site  $i$  with spin  $\sigma$ . The Hamiltonian (1) is then expressed by a sum of the Hartree-Fock Hamiltonian and the residual interactions as

$$H = H_0 + U \sum_i O_i . \quad (3)$$

Here  $O_i = \delta n_{i\uparrow} \delta n_{i\downarrow}$  and  $\delta n_{i\sigma} = n_{i\sigma} - \langle n_{i\sigma} \rangle_0$ .

In the local-ansatz approach (LA),<sup>6</sup> we take into account the Hilbert space created by operation of the residual interaction  $\{O_i\}$  onto the Hartree-Fock state  $|\phi_0\rangle$ . Introducing a variational parameter  $\eta_{\text{LA}}$  into the basis set  $\{O_i\}$ , the LA wavefunction for the ground state

is written as

$$|\Psi_{\text{LA}}\rangle = \left[ \prod_i (1 - \eta_{\text{LA}} O_i) \right] |\phi_0\rangle . \quad (4)$$

The LA is different from the Gutzwiller ansatz wavefunction  $|\Psi_{\text{GA}}\rangle = \left[ \prod_i (1 - g n_{i\uparrow} n_{i\downarrow}) \right] |\phi_0\rangle$  in which the doubly occupied states are explicitly controlled by a variational parameter  $g$ , and simplify the evaluation of the physical quantities in the weakly correlated region.

As we have emphasized in the introduction, the LA does not lead to the exact result in the small  $U$  limit because it makes use of a limited local subspace. In fact, the LA wavefunction (4) may be expanded formally in the weak interaction limit as

$$|\Psi_{\text{LA}}\rangle = |\phi_0\rangle + |\phi_1\rangle_{\text{LA}} + \cdots , \quad (5)$$

$$|\phi_1\rangle_{\text{LA}} = - \sum_i \sum_{k_1 k'_1 k_2 k'_2} \langle k'_1 | i \rangle \langle i | k_1 \rangle \langle k'_2 | i \rangle \langle i | k_2 \rangle \eta_{\text{LA}} \delta(a_{k'_2\downarrow}^\dagger a_{k_2\downarrow}) \delta(a_{k'_1\uparrow}^\dagger a_{k_1\uparrow}) |\phi_0\rangle . \quad (6)$$

Here  $\langle i | k \rangle = \exp(-i\mathbf{k} \cdot \mathbf{R}_i) / \sqrt{N}$  is an overlap integral between the localized orbital and the Bloch state with momentum  $\mathbf{k}$ ,  $\mathbf{R}_i$  denotes the atomic position, and  $N$  is the number of sites.  $a_{k\sigma}^\dagger$  ( $a_{k\sigma}$ ) denotes the creation (annihilation) operator for an electron with momentum  $\mathbf{k}$  and spin  $\sigma$ , and  $\delta(a_{k'\sigma}^\dagger a_{k\sigma}) = a_{k'\sigma}^\dagger a_{k\sigma} - \langle a_{k'\sigma}^\dagger a_{k\sigma} \rangle_0$ .

The Rayleigh-Schrödinger perturbation theory, on the other hand, yields the following form

$$|\Psi\rangle = |\phi_0\rangle + |\phi_1\rangle + \cdots , \quad (7)$$

$$|\phi_1\rangle = - \sum_i \sum_{k_1 k'_1 k_2 k'_2} \langle k'_1 | i \rangle \langle i | k_1 \rangle \langle k'_2 | i \rangle \langle i | k_2 \rangle \eta_{k'_2 k_2 k'_1 k_1}^{(0)} \delta(a_{k'_2\downarrow}^\dagger a_{k_2\downarrow}) \delta(a_{k'_1\uparrow}^\dagger a_{k_1\uparrow}) |\phi_0\rangle , \quad (8)$$

$$\eta_{k'_2 k_2 k'_1 k_1}^{(0)} = -U \lim_{z \rightarrow 0} \frac{f(\tilde{\epsilon}_{k_1\uparrow})(1 - f(\tilde{\epsilon}_{k'_1\uparrow}))f(\tilde{\epsilon}_{k_2\downarrow})(1 - f(\tilde{\epsilon}_{k'_2\downarrow}))}{z - \epsilon_{k'_1\uparrow} + \epsilon_{k_1\uparrow} - \epsilon_{k'_2\downarrow} + \epsilon_{k_2\downarrow}} . \quad (9)$$

Here  $f(\epsilon)$  is the Fermi distribution function at zero temperature, and  $\tilde{\epsilon}_{k\sigma} = \epsilon_{k\sigma} - \mu$ .  $\mu$  is the Fermi level.  $\epsilon_{k\sigma}$  is the Hartree-Fock one-electron energy eigen value given by  $\epsilon_{k\sigma} = \epsilon_0 + U\langle n_{i-\sigma} \rangle_0 + \epsilon_k - \sigma h$ , and  $\epsilon_k$  is the Fourier transform of  $t_{ij}$ .

Equation (8) compared with eq. (6) manifests that one has to take into account the momentum dependence of the variational parameters to improve the LA. We propose in the present paper the following wavefunction with momentum-dependent variational parameters  $\{\eta_{k'_2 k_2 k'_1 k_1}\}$ .

$$|\Psi\rangle = \prod_i (1 - \tilde{O}_i) |\phi_0\rangle , \quad (10)$$

$$\tilde{O}_i = \sum_{k_1 k_2 k'_1 k'_2} \langle k'_1 | i \rangle \langle i | k_1 \rangle \langle k'_2 | i \rangle \langle i | k_2 \rangle \eta_{k'_2 k_2 k'_1 k_1} \delta(a_{k'_2\downarrow}^\dagger a_{k_2\downarrow}) \delta(a_{k'_1\uparrow}^\dagger a_{k_1\uparrow}) . \quad (11)$$

The operator  $\tilde{O}_i$  is still localized on site  $i$  because of the projection  $\langle k'_1|i\rangle\langle i|k_1\rangle\langle k'_2|i\rangle\langle i|k_2\rangle$ . It should be noted that  $\tilde{O}_i^\dagger \neq \tilde{O}_i$  and  $\tilde{O}_i\tilde{O}_j \neq \tilde{O}_j\tilde{O}_i$  ( $i \neq j$ ) in general. These properties do not cause any problem when we make a single-site approximation. When we treat the nonlocal correlations we have to adopt the symmetrized wavefunction in general. The wavefunction  $|\Psi\rangle$  reduces to  $|\Psi_{\text{LA}}\rangle$  when  $\{\eta_{k'_2k_2k'_1k_1}\}$  become momentum-independent.

The variational parameters are determined by minimizing the ground-state correlation energy  $E_c$ .

$$E_c = \langle H \rangle - \langle H \rangle_0 = \frac{\langle \Psi | \tilde{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle}. \quad (12)$$

Here  $\tilde{H} = H - \langle H \rangle_0$ .

Calculation of the correlation energy with use of the new wavefunction is not easy in general. But, one can evaluate it within the single-site approximation. As shown in Appendix A, the average  $\langle \tilde{A} \rangle$  of an operator  $\tilde{A} = A - \langle A \rangle_0$  with respect to the wavefunction (10) is given in the single-site approximation as

$$\langle \tilde{A} \rangle = \sum_i \frac{\langle (1 - \tilde{O}_i^\dagger) \tilde{A} (1 - \tilde{O}_i) \rangle_0}{\langle (1 - \tilde{O}_i^\dagger)(1 - \tilde{O}_i) \rangle_0}. \quad (13)$$

By making use of the above formula, one can obtain the correlation energy per atom.

$$\epsilon_c = \frac{-\langle \tilde{O}_i^\dagger \tilde{H} \rangle_0 - \langle \tilde{H} \tilde{O}_i \rangle_0 + \langle \tilde{O}_i^\dagger \tilde{H} \tilde{O}_i \rangle_0}{1 + \langle \tilde{O}_i^\dagger \tilde{O}_i \rangle_0}. \quad (14)$$

Here we assumed that all the sites are equivalent to each other and we made use of the fact  $\langle \tilde{O}_i^\dagger \rangle_0 = \langle \tilde{O}_i \rangle_0 = 0$ .

Each term in the correlation energy (14) can be calculated by making use of Wick's theorem as follows.

$$\begin{aligned} \langle \tilde{H} \tilde{O}_i \rangle_0 &= U \sum_{k_1 k_2 k'_1 k'_2} \langle k'_1|i\rangle\langle i|k_1\rangle\langle k'_2|i\rangle\langle i|k_2\rangle \sum_j \langle k_1|j\rangle\langle j|k'_1\rangle\langle k_2|j\rangle\langle j|k'_2\rangle \\ &\quad \times \eta_{k'_2 k_2 k'_1 k_1} f(\tilde{\epsilon}_{k_1\uparrow})(1 - f(\tilde{\epsilon}_{k'_1\uparrow}))f(\tilde{\epsilon}_{k_2\downarrow})(1 - f(\tilde{\epsilon}_{k'_2\downarrow})), \end{aligned} \quad (15)$$

$$\langle \tilde{O}_i^\dagger \tilde{H} \rangle_0 = \langle \tilde{H} \tilde{O}_i \rangle_0^*, \quad (16)$$

$$\begin{aligned} \langle \tilde{O}_i^\dagger \tilde{H} \tilde{O}_i \rangle_0 &= \sum_{k_1 k_2 k'_1 k'_2} \langle i|k'_1\rangle\langle k_1|i\rangle\langle i|k'_2\rangle\langle k_2|i\rangle \eta_{k'_2 k_2 k'_1 k_1}^* \\ &\quad \times f(\tilde{\epsilon}_{k_1\uparrow})(1 - f(\tilde{\epsilon}_{k'_1\uparrow}))f(\tilde{\epsilon}_{k_2\downarrow})(1 - f(\tilde{\epsilon}_{k'_2\downarrow})) \sum_{k_3 k_4 k'_3 k'_4} \langle k'_3|i\rangle\langle i|k_3\rangle\langle k'_4|i\rangle\langle i|k_4\rangle \\ &\quad \times \left( \Delta E_{k'_2 k_2 k'_1 k_1} \delta_{k_1 k_3} \delta_{k'_1 k'_3} \delta_{k_2 k_4} \delta_{k'_2 k'_4} + U_{k'_2 k_2 k'_1 k_1 k'_4 k_4 k'_3 k_3} \right) \eta_{k'_4 k_4 k'_3 k_3}, \end{aligned} \quad (17)$$

$$\begin{aligned} U_{k'_2 k_2 k'_1 k_1 k'_4 k_4 k'_3 k_3} &= U \sum_j [\langle j|k_1\rangle\langle k_3|j\rangle f(\tilde{\epsilon}_{k_3\uparrow})\delta_{k'_1 k'_3} - \langle k'_1|j\rangle\langle j|k'_3\rangle(1 - f(\tilde{\epsilon}_{k'_3\uparrow}))\delta_{k_1 k_3}] \\ &\quad \times [\langle j|k_2\rangle\langle k_4|j\rangle f(\tilde{\epsilon}_{k_4\downarrow})\delta_{k'_2 k'_4} - \langle k'_2|j\rangle\langle j|k'_4\rangle(1 - f(\tilde{\epsilon}_{k'_4\downarrow}))\delta_{k_2 k_4}], \end{aligned} \quad (18)$$

$$\langle \tilde{O}_i^\dagger \tilde{O}_i \rangle_0 = \frac{1}{N^4} \sum_{k_1 k_2 k'_1 k'_2} |\eta_{k'_2 k_2 k'_1 k_1}|^2 f(\tilde{\epsilon}_{k_1 \uparrow})(1 - f(\tilde{\epsilon}_{k'_1 \uparrow})) f(\tilde{\epsilon}_{k_2 \downarrow})(1 - f(\tilde{\epsilon}_{k'_2 \downarrow})) . \quad (19)$$

Here  $\Delta E_{k'_2 k_2 k'_1 k_1} = \epsilon_{k'_2 \downarrow} - \epsilon_{k_2 \downarrow} + \epsilon_{k'_1 \uparrow} - \epsilon_{k_1 \uparrow}$  is a two-particle excitation energy.

The above expressions (15) and (18) contain nonlocal terms in the summation over  $j$  (*i.e.*,  $\sum_j$ ). We thus make additional single-site approximation called the  $R = 0$  approximation.<sup>21</sup> In eq. (15), for example, we have

$$\sum_j \langle k'_1 | i \rangle \langle i | k_1 \rangle \langle k'_2 | i \rangle \langle i | k_2 \rangle \langle k_1 | j \rangle \langle j | k'_1 \rangle \langle k_2 | j \rangle \langle j | k'_2 \rangle = \frac{1}{N^4} \sum_j e^{i(k_1 + k_2 - k'_1 - k'_2)(R_j - R_i)} . \quad (20)$$

The  $R = 0$  approximation only takes into account the local term ( $j = i$ ) in the above summation, so that  $\langle \tilde{H} \tilde{O}_i \rangle_0 (= \langle \tilde{O}_i^\dagger \tilde{H} \rangle_0^*)$ , and  $\langle \tilde{O}_i^\dagger \tilde{H} \tilde{O}_i \rangle_0$  reduce as follows.

$$\langle \tilde{H} \tilde{O}_i \rangle_0 = \frac{U}{N^4} \sum_{k_1 k_2 k'_1 k'_2} f(\tilde{\epsilon}_{k_1 \uparrow})(1 - f(\tilde{\epsilon}_{k'_1 \uparrow})) f(\tilde{\epsilon}_{k_2 \downarrow})(1 - f(\tilde{\epsilon}_{k'_2 \downarrow})) \eta_{k'_2 k_2 k'_1 k_1} , \quad (21)$$

$$\begin{aligned} \langle \tilde{O}_i^\dagger \tilde{H} \tilde{O}_i \rangle_0 &= \frac{1}{N^4} \sum_{k_1 k_2 k'_1 k'_2} f(\tilde{\epsilon}_{k_1 \uparrow})(1 - f(\tilde{\epsilon}_{k'_1 \uparrow})) f(\tilde{\epsilon}_{k_2 \downarrow})(1 - f(\tilde{\epsilon}_{k'_2 \downarrow})) \eta_{k'_2 k_2 k'_1 k_1}^* \\ &\quad \times \left[ \Delta E_{k'_2 k_2 k'_1 k_1} \eta_{k'_2 k_2 k'_1 k_1} \right. \\ &\quad + \frac{U}{N^2} \left\{ \sum_{k_3 k_4} f(\tilde{\epsilon}_{k_3 \uparrow}) f(\tilde{\epsilon}_{k_4 \downarrow}) \eta_{k'_2 k_4 k'_1 k_3} - \sum_{k_3 k'_4} f(\tilde{\epsilon}_{k_3 \uparrow})(1 - f(\tilde{\epsilon}_{k'_4 \downarrow})) \eta_{k'_4 k_2 k'_1 k_3} \right. \\ &\quad \left. \left. - \sum_{k'_3 k_4} (1 - f(\tilde{\epsilon}_{k'_3 \uparrow})) f(\tilde{\epsilon}_{k_4 \downarrow}) \eta_{k'_2 k_4 k'_3 k_1} + \sum_{k'_3 k'_4} (1 - f(\tilde{\epsilon}_{k'_3 \uparrow}))(1 - f(\tilde{\epsilon}_{k'_4 \downarrow})) \eta_{k'_4 k_2 k'_3 k_1} \right\} \right] . \quad (22) \end{aligned}$$

Variational parameters  $\{\eta_{k'_2 k_2 k'_1 k_1}\}$  are obtained by minimizing the correlation energy  $\epsilon_c$ , *i.e.*, eq. (14) with eqs. (19), (21), and (22). The self-consistent equations for  $\{\eta_{k'_2 k_2 k'_1 k_1}\}$  in the single-site approximation are given as follows.

$$\begin{aligned} &(\Delta E_{k'_2 k_2 k'_1 k_1} - \epsilon_c) \eta_{k'_2 k_2 k'_1 k_1} \\ &+ \frac{U}{N^2} \left[ \sum_{k_3 k_4} f(\tilde{\epsilon}_{k_3 \uparrow}) f(\tilde{\epsilon}_{k_4 \downarrow}) \eta_{k'_2 k_4 k'_1 k_3} - \sum_{k_3 k'_4} f(\tilde{\epsilon}_{k_3 \uparrow})(1 - f(\tilde{\epsilon}_{k'_4 \downarrow})) \eta_{k'_4 k_2 k'_1 k_3} \right. \\ &\quad \left. - \sum_{k'_3 k_4} (1 - f(\tilde{\epsilon}_{k'_3 \uparrow})) f(\tilde{\epsilon}_{k_4 \downarrow}) \eta_{k'_2 k_4 k'_3 k_1} + \sum_{k'_3 k'_4} (1 - f(\tilde{\epsilon}_{k'_3 \uparrow}))(1 - f(\tilde{\epsilon}_{k'_4 \downarrow})) \eta_{k'_4 k_2 k'_3 k_1} \right] = U . \quad (23) \end{aligned}$$

Note that  $\eta_{k'_2 k_2 k'_1 k_1}$  should vanish when  $U \rightarrow 0$ . Thus in the weak  $U$  limit, one can omit the second term at the l.h.s. (left-hand-side) of eq. (23). We then obtain the solution in the weak  $U$  limit as

$$\eta_{k'_2 k_2 k'_1 k_1} = \frac{U}{\Delta E_{k'_2 k_2 k'_1 k_1}} . \quad (24)$$

In the atomic limit,  $\Delta E_{k'_2 k_2 k'_1 k_1} = 0$ . We find then a  $k$ -independent solution being identical

with the LA.

$$\eta_{\text{LA}} = \frac{-\langle O_i \tilde{H} O_i \rangle_0 + \sqrt{\langle O_i \tilde{H} O_i \rangle_0^2 + 4\langle O_i \tilde{H} \rangle_0^2 \langle O_i^2 \rangle_0}}{2\langle O_i \tilde{H} \rangle_0 \langle O_i^2 \rangle_0}. \quad (25)$$

It is not easy to find the solution of eq. (23) for the intermediate strength of Coulomb interaction  $U$ . We therefore consider an approximate solution which interpolates between the weak and the atomic limits. Note that the second term at the l.h.s. of eq. (23) do not affect the solution in the weakly correlated limit as we have mentioned. Therefore we approximate  $\{\eta_{k'_2 k_2 k'_1 k_1}\}$  in the second term with the momentum-independent parameter  $\eta$  which is suitable for the atomic region. We have then an approximate solution as follows.

$$\eta_{k'_2 k_2 k'_1 k_1} = \frac{U[1 - \eta(1 - 2\langle n_{i\uparrow} \rangle_0)(1 - 2\langle n_{i\downarrow} \rangle_0)]}{\Delta E_{k'_2 k_2 k'_1 k_1} - \epsilon_c}. \quad (26)$$

The best value of  $\eta$  should be determined variationally, but we make use of that in the LA for simplicity. Furthermore, we approximate  $\epsilon_c$  in the denominator of eq. (26) with the correlation energy in the LA.

Substituting the variational parameters (26) into eq. (14), we obtain the ground-state correlation energy. The each element in the energy is given as follows.

$$\begin{aligned} \langle \tilde{H} \tilde{O}_i \rangle_0 &= \langle \tilde{O}_i^\dagger \tilde{H} \rangle_0^* \\ &= U^2[1 - \eta(1 - 2\langle n_{i\uparrow} \rangle_0)(1 - 2\langle n_{i\downarrow} \rangle_0)] \\ &\times \int \frac{[\prod_n d\epsilon_n] \rho_\uparrow(\epsilon_1) \rho_\uparrow(\epsilon_2) \rho_\downarrow(\epsilon_3) \rho_\downarrow(\epsilon_4) f(\epsilon_1)(1 - f(\epsilon_2))f(\epsilon_3)(1 - f(\epsilon_4))}{\epsilon_4 - \epsilon_3 + \epsilon_2 - \epsilon_1 - \epsilon_c}, \end{aligned} \quad (27)$$

$$\langle \tilde{O}_i^\dagger \tilde{H} \tilde{O}_i \rangle_0 = \langle \tilde{O}_i^\dagger \tilde{H}_0 \tilde{O}_i \rangle_0 + U \langle \tilde{O}_i^\dagger O_i \tilde{O}_i \rangle_0, \quad (28)$$

$$\begin{aligned} \langle \tilde{O}_i^\dagger \tilde{H}_0 \tilde{O}_i \rangle_0 &= U^2[1 - \eta(1 - 2\langle n_{i\uparrow} \rangle_0)(1 - 2\langle n_{i\downarrow} \rangle_0)]^2 \\ &\times \int \left[ \prod_n d\epsilon_n \right] \rho_\uparrow(\epsilon_1) \rho_\uparrow(\epsilon_2) \rho_\downarrow(\epsilon_3) \rho_\downarrow(\epsilon_4) \\ &\times f(\epsilon_1)(1 - f(\epsilon_2))f(\epsilon_3)(1 - f(\epsilon_4)) \frac{\epsilon_4 - \epsilon_3 + \epsilon_2 - \epsilon_1}{(\epsilon_4 - \epsilon_3 + \epsilon_2 - \epsilon_1 - \epsilon_c)^2}, \end{aligned} \quad (29)$$

$$\begin{aligned} \langle \tilde{O}_i^\dagger O_i \tilde{O}_i \rangle_0 &= U^2[1 - \eta(1 - 2\langle n_{i\uparrow} \rangle_0)(1 - 2\langle n_{i\downarrow} \rangle_0)]^2 \\ &\times \int \left[ \prod_n d\epsilon_n \right] \rho_\uparrow(\epsilon_1) \rho_\uparrow(\epsilon_2) \rho_\downarrow(\epsilon_3) \rho_\downarrow(\epsilon_4) \frac{f(\epsilon_1)(1 - f(\epsilon_2))f(\epsilon_3)(1 - f(\epsilon_4))}{\epsilon_4 - \epsilon_3 + \epsilon_2 - \epsilon_1 - \epsilon_c} \\ &\times \left[ \int \frac{d\epsilon_5 d\epsilon_6 \rho_\uparrow(\epsilon_5) \rho_\downarrow(\epsilon_6) f(\epsilon_5) f(\epsilon_6)}{\epsilon_4 - \epsilon_6 + \epsilon_2 - \epsilon_5 - \epsilon_c} - \int \frac{d\epsilon_5 d\epsilon_6 \rho_\uparrow(\epsilon_5) \rho_\downarrow(\epsilon_6) f(\epsilon_5)(1 - f(\epsilon_6))}{\epsilon_6 - \epsilon_3 + \epsilon_2 - \epsilon_5 - \epsilon_c} \right. \\ &\left. - \int \frac{d\epsilon_5 d\epsilon_6 \rho_\uparrow(\epsilon_5) \rho_\downarrow(\epsilon_6)(1 - f(\epsilon_5))f(\epsilon_6)}{\epsilon_4 - \epsilon_6 + \epsilon_5 - \epsilon_1 - \epsilon_c} + \int \frac{d\epsilon_5 d\epsilon_6 \rho_\uparrow(\epsilon_5) \rho_\downarrow(\epsilon_6)(1 - f(\epsilon_5))(1 - f(\epsilon_6))}{\epsilon_6 - \epsilon_3 + \epsilon_5 - \epsilon_1 - \epsilon_c} \right], \end{aligned} \quad (30)$$

$$\langle \tilde{O}_i^\dagger \tilde{O}_i \rangle_0 = U^2[1 - \eta(1 - 2\langle n_{i\uparrow} \rangle_0)(1 - 2\langle n_{i\downarrow} \rangle_0)]^2$$

$$\times \int \left[ \prod_n d\epsilon_n \right] \rho_{\uparrow}(\epsilon_1) \rho_{\uparrow}(\epsilon_2) \rho_{\downarrow}(\epsilon_3) \rho_{\downarrow}(\epsilon_4) \frac{f(\epsilon_1)(1-f(\epsilon_2))f(\epsilon_3)(1-f(\epsilon_4))}{(\epsilon_4 - \epsilon_3 + \epsilon_2 - \epsilon_1 - \epsilon_c)^2}. \quad (31)$$

Here  $\rho_{\sigma}(\epsilon)$  is the density of states for the Hartree-Fock one-electron energy eigen values measured from the Fermi level.

Electron number  $\langle n_i \rangle (= \sum_{\sigma} \langle n_{i\sigma} \rangle)$ , the momentum distribution  $\langle n_{k\sigma} \rangle$ , and the double occupation number  $\langle n_{i\uparrow} n_{i\downarrow} \rangle$  are obtained from  $\partial \langle H \rangle / \partial \epsilon$ ,  $\partial \langle H \rangle / \partial \hat{\epsilon}_{k\sigma}$ , and  $\partial \langle H \rangle / \partial U_i$ , respectively. Here  $\hat{\epsilon}_{k\sigma} = \epsilon_k - \sigma h$  and  $\epsilon_k$  is the Fourier transform of  $t_{ij}$ . Making use of the single-site energy (14) and the Feynman-Hellmann theorem, we obtain the following expressions.

$$\langle n_i \rangle = \langle n_i \rangle_0 + \frac{\langle \tilde{O}_i \tilde{n}_i \tilde{O}_i \rangle_0}{1 + \langle \tilde{O}_i^{\dagger} \tilde{O}_i \rangle_0}, \quad (32)$$

$$\langle n_{k\sigma} \rangle = \langle n_{k\sigma} \rangle_0 + \frac{N \langle \tilde{O}_i \tilde{n}_{k\sigma} \tilde{O}_i \rangle_0}{1 + \langle \tilde{O}_i^{\dagger} \tilde{O}_i \rangle_0}, \quad (33)$$

$$\langle n_{i\uparrow} n_{i\downarrow} \rangle = \langle n_{i\uparrow} \rangle_0 \langle n_{i\downarrow} \rangle_0 + \frac{-\langle \tilde{O}_i^{\dagger} \tilde{O}_i \rangle_0 - \langle O_i \tilde{O}_i \rangle_0 + \langle \tilde{O}_i^{\dagger} O_i \tilde{O}_i \rangle_0 + \sum_{\sigma} \langle n_{i-\sigma} \rangle_0 \langle \tilde{O}_i^{\dagger} \tilde{n}_{i\sigma} \tilde{O}_i \rangle_0}{1 + \langle \tilde{O}_i^{\dagger} \tilde{O}_i \rangle_0}. \quad (34)$$

Here  $\tilde{n}_i = n_i - \langle n_i \rangle_0$ ,  $\tilde{n}_{k\sigma} = n_{k\sigma} - \langle n_{k\sigma} \rangle_0$ , and

$$\begin{aligned} \langle \tilde{O}_i^{\dagger} \tilde{n}_{i\sigma} \tilde{O}_i \rangle_0 &= 2U^2 [1 - \eta(1 - 2\langle n_{i\uparrow} \rangle_0)(1 - 2\langle n_{i\downarrow} \rangle_0)]^2 \\ &\times \int \left[ \prod_n d\epsilon_n \right] \frac{\rho_{-\sigma}(\epsilon_1) \rho_{-\sigma}(\epsilon_2) \rho_{\sigma}(\epsilon_3) \rho_{\sigma}(\epsilon_4) \rho_{\sigma}(\epsilon_5) f(\epsilon_1)(1-f(\epsilon_2))f(\epsilon_3)(1-f(\epsilon_4))}{\epsilon_4 - \epsilon_3 + \epsilon_2 - \epsilon_1 - \epsilon_c} \\ &\times \left[ \frac{1 - f(\epsilon_5)}{\epsilon_5 - \epsilon_3 + \epsilon_2 - \epsilon_1 - \epsilon_c} - \frac{f(\epsilon_5)}{\epsilon_4 - \epsilon_5 + \epsilon_2 - \epsilon_1 - \epsilon_c} \right], \end{aligned} \quad (35)$$

$$\begin{aligned} N \langle \tilde{O}_i^{\dagger} \tilde{n}_{k\sigma} \tilde{O}_i \rangle_0 &= U^2 [1 - \eta(1 - 2\langle n_{i\uparrow} \rangle_0)(1 - 2\langle n_{i\downarrow} \rangle_0)]^2 \\ &\times \left[ (1 - f(\epsilon_{k\sigma})) \int \frac{d\epsilon_1 d\epsilon_2 d\epsilon_3 \rho_{-\sigma}(\epsilon_1) \rho_{-\sigma}(\epsilon_2) \rho_{\sigma}(\epsilon_3) f(\epsilon_1)(1-f(\epsilon_2))f(\epsilon_3)}{(\epsilon_1 - \epsilon_2 + \epsilon_{k\sigma} - \epsilon_3 - \epsilon_c)^2} \right. \\ &\left. - f(\epsilon_{k\sigma}) \int \frac{d\epsilon_1 d\epsilon_2 d\epsilon_3 \rho_{-\sigma}(\epsilon_1) \rho_{-\sigma}(\epsilon_2) \rho_{\sigma}(\epsilon_3) f(\epsilon_1)(1-f(\epsilon_2))(1-f(\epsilon_3))}{(\epsilon_1 - \epsilon_2 + \epsilon_3 - \epsilon_{k\sigma} - \epsilon_c)^2} \right], \end{aligned} \quad (36)$$

$$\begin{aligned} \langle \tilde{O}_i^{\dagger} O_i \rangle_0 + \langle O_i \tilde{O}_i \rangle_0 &= 2U [1 - \eta(1 - 2\langle n_{i\uparrow} \rangle_0)(1 - 2\langle n_{i\downarrow} \rangle_0)] \\ &\times \int \frac{[\prod_n d\epsilon_n] \rho_{\uparrow}(\epsilon_1) \rho_{\uparrow}(\epsilon_2) \rho_{\downarrow}(\epsilon_3) \rho_{\downarrow}(\epsilon_4) f(\epsilon_1)(1-f(\epsilon_2))f(\epsilon_3)(1-f(\epsilon_4))}{\epsilon_4 - \epsilon_3 + \epsilon_2 - \epsilon_1 - \epsilon_c}. \end{aligned} \quad (37)$$

It should be noted that the expressions of these physical quantities consist of the multiple integrals up to the 6-folds. One can reduce these integrals up to the 2-folds using the Laplace transform. Their expressions are given in Appendix B.

### 3. Numerical Example: Half-Filled Hubbard Model

We have performed the numerical calculations of the half-filled band Hubbard model in order to examine the properties of the local ansatz with momentum-dependent variational parameters (MLA). We consider here the hypercubic lattice in infinite dimensions, where the



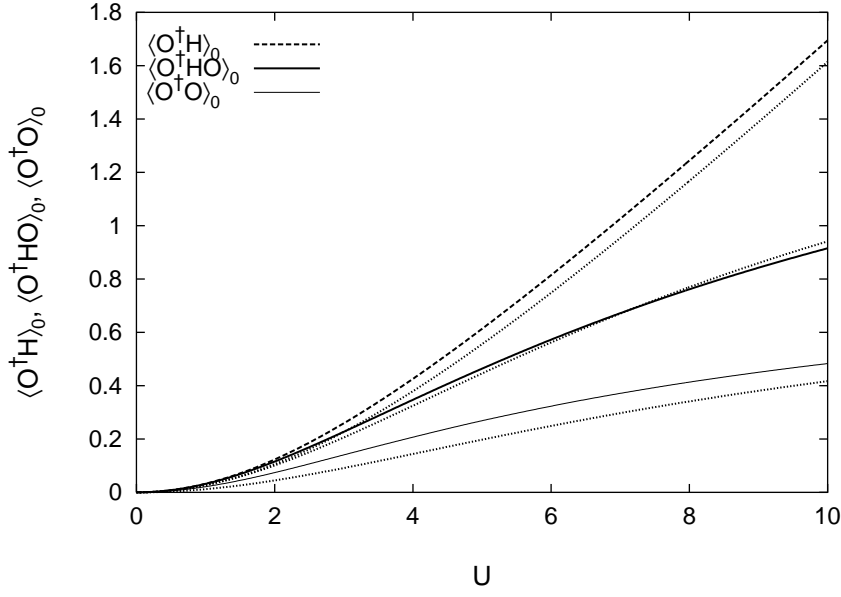


Fig. 1. Calculated elements  $\langle \tilde{O}_i^\dagger \tilde{H} \rangle_0$  (dashed curve),  $\langle \tilde{O}_i^\dagger \tilde{H} \tilde{O}_i \rangle_0$  (solid curve), and  $\langle \tilde{O}_i^\dagger \tilde{O}_i \rangle_0$  (thin solid curve) as a function of the Coulomb interaction parameter  $U$ . Corresponding curves in the LA are shown by dotted curves.

single-site approximation works best. The density of states for noninteracting system on the hypercubic lattice is given by  $\rho(\epsilon) = (1/\sqrt{\pi}) \exp(-\epsilon^2)$ , in which the energy unit is chosen to be  $\int d\epsilon \rho(\epsilon) \epsilon^2 = 1/2$ .

Figure 1 shows the curves for  $\langle \tilde{O}_i^\dagger \tilde{H} \rangle_0$ ,  $\langle \tilde{O}_i^\dagger \tilde{H} \tilde{O}_i \rangle_0$ , and  $\langle \tilde{O}_i^\dagger \tilde{O}_i \rangle_0$  in the correlation energy as a function of the Coulomb interaction energy parameter  $U$ . These are proportional to  $U^2$  in the small  $U$  limit. The energy  $\langle \tilde{O}_i^\dagger \tilde{H} \rangle_0$  agrees with  $\langle \tilde{O}_i^\dagger \tilde{H} \tilde{O}_i \rangle_0$  in the small  $U$  limit as is verified from eqs. (27) and (28). This implies that  $\epsilon_c \approx -\langle \tilde{O}_i^\dagger \tilde{H} \rangle_0$  in the small  $U$  limit. For large  $U$ , the energy  $\langle \tilde{O}_i^\dagger \tilde{H} \tilde{O}_i \rangle_0$  becomes smaller than  $\langle \tilde{O}_i^\dagger \tilde{H} \rangle_0$  because the former changes with  $\{\eta_{k'_2 k_2 k'_1 k_1}\}$  in a quadratic way, while the latter linearly depends on  $U$  as  $U \eta_{k'_2 k_2 k'_1 k_1}$ , and because  $\{\eta_{k'_2 k_2 k'_1 k_1}\}$  saturate when  $U$  is large. The renormalization contribution  $\langle \tilde{O}_i^\dagger \tilde{O}_i \rangle_0$  tends to saturate with increasing  $U$  because of the same reason. As a consequence, the energy  $-\langle \tilde{O}_i^\dagger \tilde{H} \rangle_0$  forms the leading term in the correlation energy even for large  $U$ .

The same quantities in the LA are obtained by the replacements  $\eta_{k'_2 k_2 k'_1 k_1} \rightarrow \eta_{\text{LA}}$ ;  $\langle \tilde{O}_i^\dagger \tilde{H} \rangle_0 \rightarrow \eta_{\text{LA}} \langle O_i \tilde{H} \rangle_0$ ,  $\langle \tilde{O}_i^\dagger \tilde{H} \tilde{O}_i \rangle_0 \rightarrow \eta_{\text{LA}}^2 \langle O_i \tilde{H} O_i \rangle_0$ , and  $\langle \tilde{O}_i^\dagger \tilde{O}_i \rangle_0 \rightarrow \eta_{\text{LA}}^2 \langle O_i^2 \rangle_0$  in eqs. (27), (28), and (31). Their expressions are calculated analytically in the present case as  $\eta_{\text{LA}} \langle O_i \tilde{H} \rangle_0 = \eta_{\text{LA}} U/16$ ,  $\eta_{\text{LA}}^2 \langle O_i \tilde{H} O_i \rangle_0 = \eta_{\text{LA}}^2/4\sqrt{\pi}$ ,  $\eta_{\text{LA}}^2 \langle O_i^2 \rangle_0 = \eta_{\text{LA}}^2/16$ , and

$$\eta_{\text{LA}} = \frac{-\frac{1}{\sqrt{\pi}} + \sqrt{\frac{1}{\pi} + \frac{U^2}{16}}}{\frac{U}{32}}. \quad (38)$$

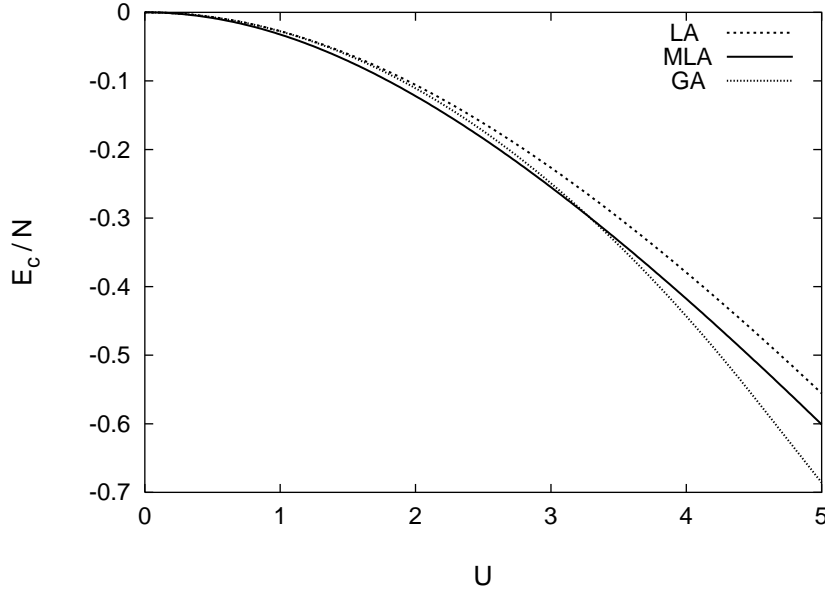


Fig. 2. The correlation energies vs. Coulomb interaction energy parameter  $U$  in the LA (dashed curve), the MLA (solid curve), and the GA (dotted curve).

These quantities in the LA are also presented in Fig. 1 by dotted curves. The results in the LA describe those in the MLA rather well over a wide range of the Coulomb interaction. It should be noted that the curves in the LA deviate from those in the MLA even in the small  $U$  limit. A remarkable point is that  $\langle \tilde{O}_i^\dagger \tilde{H} \rangle_0$  is larger than that in the LA. This lowers the ground-state energy of the MLA.

Figure 2 shows calculated correlation energy as a function of Coulomb interaction. The energy in the MLA is lower than that of the LA over all Coulomb interaction energy parameters  $U$ , verifying an improvement of the wavefunction. Moreover, the MLA wavefunction leads to the correlation energy lower than that of the original Gutzwiller Ansatz (GA) for the Coulomb interaction energy parameter  $U \leq U^* = 3.28$ . We can expect that the MLA yields better results in the interaction range  $[0, U^*]$ , while the original GA should be better for  $U \geq U^*$ .

We present the double occupation number vs. Coulomb interaction curves in Fig. 3. The double occupancy in the uncorrelated limit is  $1/4$ , and decreases with increasing Coulomb interaction  $U$ . Both the LA and the MLA yield  $\langle n_{i\uparrow} n_{i\downarrow} \rangle = 0$  in the limit  $U = \infty$ . The MLA suppresses  $\langle n_{i\uparrow} n_{i\downarrow} \rangle$  of the LA typically by about 10 % in the intermediate regime of Coulomb interaction. The double occupation number in the GA linearly decreases with increasing  $U$  and causes the metal-insulator transition at  $U_{c2} = 8/\sqrt{\pi} (= 4.51)$ . The GA underestimates the double occupancy in the insulator regime because  $\langle n_{i\uparrow} n_{i\downarrow} \rangle$  should be finite even beyond  $U_{c2}$  due to virtual exchange of electrons between the nearest neighbor atoms. Present result of the MLA indicates that the GA overestimates  $\langle n_{i\uparrow} n_{i\downarrow} \rangle$  for small  $U (\lesssim 2)$  and underestimates it at  $U \sim 3$ .

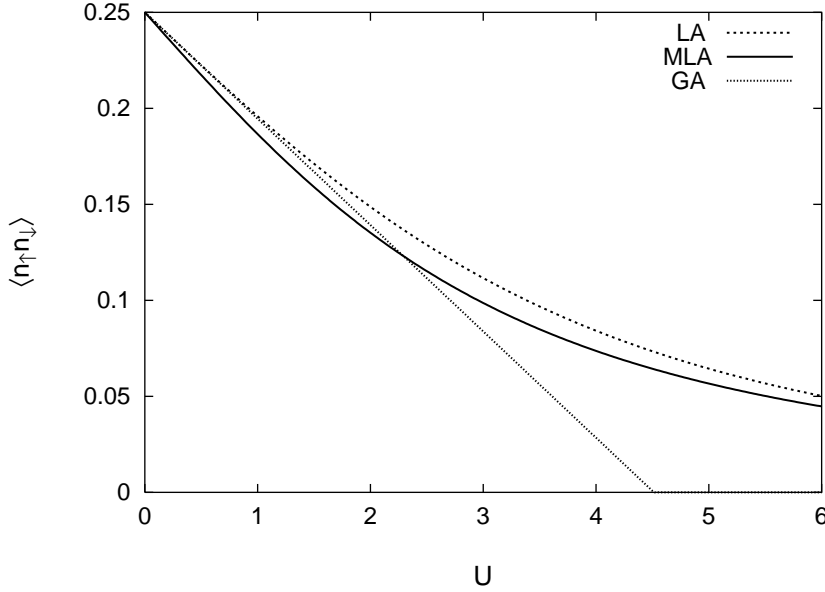


Fig. 3. The double occupation number vs. Coulomb interaction energy  $U$  curves in the LA (dashed curve), the MLA (solid curve), and the GA (dotted curve).

The difference between the LA and the MLA is seen more clearly in the momentum-dependent quantities. Figure 4 shows the momentum distribution in various approximations. The distributions in the LA are constant below and above the Fermi level irrespective of  $U$ . This behavior is also found in the GA.<sup>2</sup> The MLA shows a distinct momentum dependence of  $\langle n_{k\sigma} \rangle$  via the energy  $\epsilon_k$ . The results are in good agreement with those in the previous results of the RPT-1 (The first-order approximation in the renormalized perturbation theory) in the projection operator method CPA.<sup>8</sup> The latter is exact up to the second order in  $U$ , and reproduce the Hubbard III approximation in the large  $U$  region.

The jump at the Fermi level in the momentum distribution gives us the quasiparticle weight  $Z$  (*i.e.* the inverse effective mass). Calculated quasiparticle weight vs. Coulomb interaction curves are shown in Fig. 5. The quasiparticle weight in the LA changes as  $Z = (1 - 3\eta_{\text{LA}}^2/16)/(1 + \eta_{\text{LA}}^2/16)$  and vanishes at  $U_{c2}(\text{LA}) = 24/\sqrt{3\pi} (= 7.82)$ . In the GA,<sup>3</sup> the quasiparticle weight changes as  $Z = 1 - (U/U_{c2})^2$ . The curve in the GA agrees with the LA curve for small  $U$ . But it deviates from the LA when  $U$  becomes large, and vanishes at  $U_{c2}(\text{GA}) = 8/\sqrt{\pi} (= 4.51)$ . It should be noted that the GA curve strongly deviates from the curve in the NRG<sup>20</sup> which is considered to be the best at present. The quasiparticle weight in the MLA much improves the LA; it is close to the curve in the NRG up to  $U \approx 2.5$ , and vanishes at  $U_{c2}(\text{MLA}) = 3.21$ . The latter should be compared with  $U_{c2}(\text{NRG}) = 4.10$ . We note that the wavefunction itself does not show the metal-insulator transition at  $U_{c2}$  in the present approximation because the approximate expression of variational parameters (26) has no singularity at finite value of  $U$ . In this sense, the calculated  $Z$  and wavefunction are not

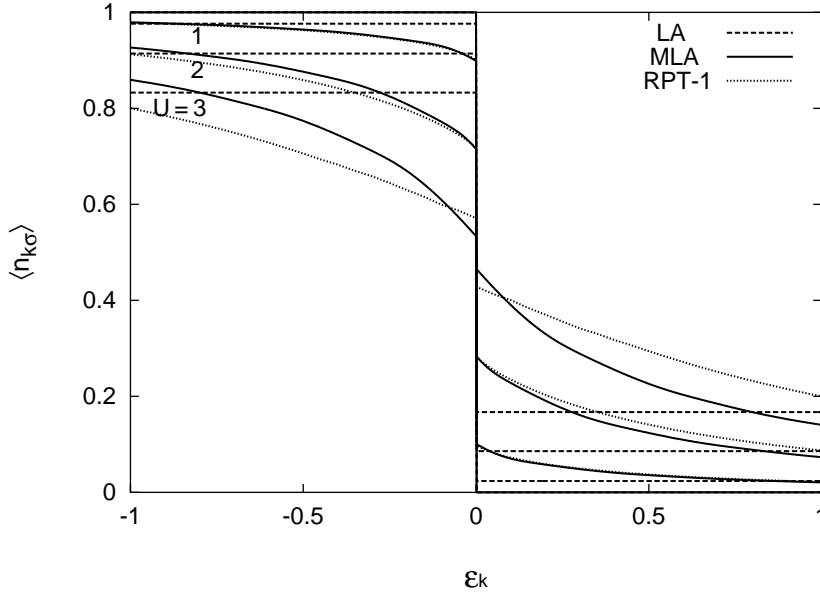


Fig. 4. The momentum distribution curves as a function of energy  $\epsilon_k$  for various Coulomb interaction energy parameters  $U$ . The results of the LA: dashed curves, the MLA: solid curves, and the RPT-1: dotted curves.<sup>8</sup>

self-consistent in the present approximation. The values of  $Z$  obtained by the LA and MLA should be regarded as an estimate from the metallic side.

#### 4. Application to Excitation Spectra

We demonstrate in this section that the present approach is also useful for understanding the correlation effects on excitation spectra. This can be made by combining the MLA with the projection operator method (see, for example, Chap. 6 in Ref. 7). The projection technique treats the dynamics of electrons and the static average separately, and the latter can be calculated by using the wavefunction method.

We adopt again the half-filled band Hubbard model in infinite dimensions, and apply the projection operator CPA method (PM-CPA).<sup>8</sup> In this methods, we describe the single-particle excitations by means of the Fourier transform of the retarded Green function,  $(a_{i\sigma}^\dagger | (z - L)^{-1} a_{j\sigma}^\dagger)$ . Here the Liouville operator  $L$  defined by  $LA = [H, A]_-$  for an operator  $A$  describes the dynamics of electrons,  $z = \omega + i\delta$ ,  $\delta$  is an infinitesimal positive number, and the inner product between the operators  $A$  and  $B$  is defined by  $(A|B) = \langle [A^\dagger, B]_+ \rangle$ . We approximate in the PM-CPA the operator  $L$  by an energy dependent Liouvillean  $\tilde{L}(z)$  for an effective Hamiltonian with a coherent potential  $\tilde{\Sigma}(z)$ ,  $\sum_{i\sigma} \tilde{\Sigma}(z) n_{i\sigma} + \sum_{ij\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma}$ . The Green function for  $\tilde{L}(z)$  is given by

$$F(z) = \int \frac{\rho(\epsilon) d\epsilon}{z - \tilde{\Sigma}(z) - \epsilon}. \quad (39)$$

Here  $\rho(\epsilon)$  is the density of states (DOS) per site for the noninteracting system.

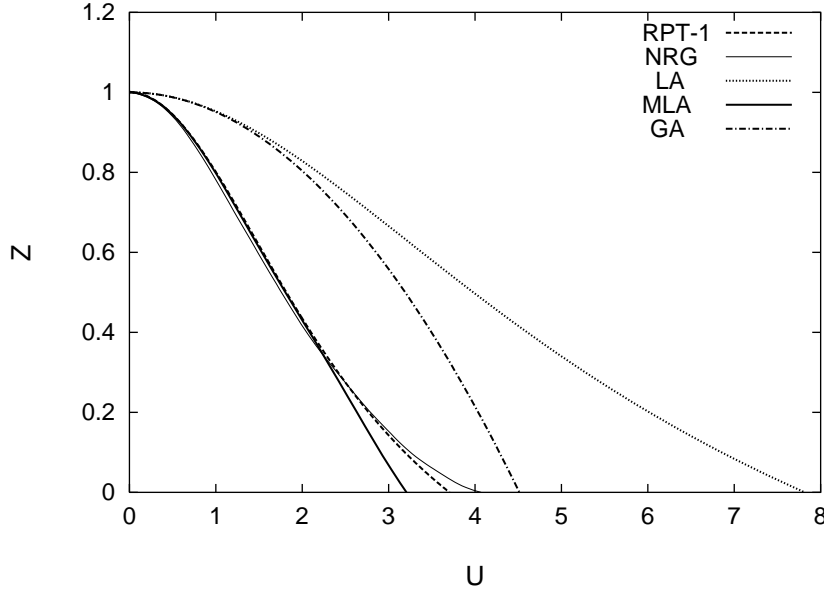


Fig. 5. Quasiparticle-weight vs. Coulomb interaction curves in various theories. The RPT-1: dashed curve, the NRG: thin solid curve,<sup>20</sup> the LA: dotted curve, the MLA: solid curve, and the GA: dot-dashed curve.<sup>3</sup>

To obtain the coherent potential  $\tilde{\Sigma}(z)$ , we consider an impurity system with Coulomb interaction on a site embedded in the coherent potential. The site-diagonal impurity Green function for the system is then given by

$$G^{(i)}(z) = \left( F(z)^{-1} - \tilde{\Lambda}^{(i)}(z) + \tilde{\Sigma}(z) \right)^{-1}. \quad (40)$$

The self-energy  $\tilde{\Lambda}^{(i)}(z)$  is expressed as follows for the half-filled band according to the RPT (Renormalized Perturbation Theory).<sup>8</sup>

$$\tilde{\Lambda}^{(i)}(z) = \frac{U^2 \overline{G}_0^{(i)}(z)}{1 + 4\tilde{\Sigma}(z) \overline{G}_0^{(i)}(z)}, \quad (41)$$

$$\overline{G}_0^{(i)}(z) = (A_{i\sigma}^\dagger | (z - \overline{L}_0(z) - \overline{L}_I^{(i)}(z) \overline{Q})^{-1} A_{i\sigma}^\dagger). \quad (42)$$

Here  $A_{i\sigma}^\dagger \equiv a_{i\sigma}^\dagger \delta n_{i-\sigma}$  is an atomic operator expanded by the intra-atomic Coulomb interaction.  $\overline{L}_0(z) = Q \tilde{L}(z) Q$  and  $\overline{L}_I^{(i)}(z) = Q L_I^{(i)}(z) Q$  are respectively the coherent Liouville operator and the interaction Liouville operator in which  $L_I^{(i)}(z)$  is defined by  $L_I^{(i)}(z) A = [U \delta n_{i\uparrow} \delta n_{i\downarrow} - \sum_\sigma \tilde{\Sigma}(z) n_{i\sigma}, A]$ . Operator  $Q$  ( $\overline{Q}$ ) denotes a projection operator which removes the original operator space  $\{|a_{i\sigma}^\dagger\rangle\}$  (the atomic operator space  $\{|A_{i\sigma}^\dagger\rangle\}$ ). Note that the above expression (41) is exact, and  $\overline{G}_0^{(i)}(z)$  denotes a screened memory function in which the dynamics for the strong atomic excitations have been removed.

We consider here the lowest-order approximation (RPT-0)<sup>8</sup>; we neglect in  $\overline{G}_0^{(i)}(z)$  a ‘weak’ interaction Liouvillean  $\overline{L}_I^{(i)}(z) \overline{Q}$ . Expanding the operator  $A_{i\sigma}^\dagger$  by means of the nonlocal oper-

ators  $\{a_{k\sigma}^\dagger \delta(a_{k'-\sigma}^\dagger a_{k''-\sigma})\}$  as  $\sum_{kk'k''} a_{k\sigma}^\dagger \delta(a_{k'-\sigma}^\dagger a_{k''-\sigma}) \langle k|i \rangle \langle k'|i \rangle \langle i|k'' \rangle$ , we reach a simple form of the screened memory function as follows (see eq. (74) in Ref. 8).

$$\bar{G}_0^{(i)}(z) = \int \frac{d\epsilon d\epsilon' d\epsilon'' \rho(\epsilon) \rho(\epsilon') \rho(\epsilon'') X(\epsilon, \epsilon', \epsilon'')}{z - \tilde{\Sigma}(z) - \epsilon - \epsilon' + \epsilon''}. \quad (43)$$

Here we have omitted the spin dependence for simplicity. The correlation function  $X(\epsilon, \epsilon', \epsilon'')$  is given by

$$\begin{aligned} X(\epsilon_k, \epsilon_{k'}, \epsilon_{k''}) &= \sum_{k'_1 k''_1} e^{i(k' - k'' - k'_1 + k''_1) \cdot R_i} \langle \delta(a_{k'-\sigma}^\dagger a_{k''-\sigma}) \delta(a_{k'_1-\sigma}^\dagger a_{k''_1-\sigma}) \rangle \\ &+ \sum_{k_1 k''_1} e^{i(k - k'' - k_1 + k''_1) \cdot R_i} \langle a_{k'_1-\sigma}^\dagger a_{k''-\sigma} a_{k_1\sigma} a_{k''_1\sigma}^\dagger \rangle \\ &- \sum_{k_1 k'_1} e^{i(k + k' - k_1 - k'_1) \cdot R_i} \langle a_{k'-\sigma}^\dagger a_{k'_1-\sigma} a_{k_1\sigma} a_{k''_1\sigma}^\dagger \rangle. \end{aligned} \quad (44)$$

The function  $X$  should depend on the momentum only via  $\epsilon_k$ , an one-electron eigenvalue in the Hartree-Fock approximation.

The coherent potential  $\tilde{\Sigma}(z)$  is obtained from a self-consistent condition (*i.e.*, the CPA equation<sup>9,10</sup>);

$$G^{(i)}(z) = F(z). \quad (45)$$

Note that eq. (43) reduces to the second order self-energy when  $X(\epsilon, \epsilon', \epsilon'')$  is treated by the Hartree-Fock approximation. Thus, the self-energy (41) yields the exact weak Coulomb interaction limit. The self-energy (41) also becomes exact in the atomic limit.

In order to obtain the explicit expression for the self-energy from eq. (44), we adopted in our previous paper<sup>8</sup> the Hartree-Fock wave function. We adopt here the new wavefunction (10) and the single-site approximation (*i.e.*,  $R = 0$  approximation<sup>21</sup>). We have calculated the function  $X(\epsilon_k, \epsilon_{k'}, \epsilon_{k''})$  in eq. (43). Actual expressions used in the numerical calculations are given in Appendix C. The RPT-0 memory function obtained from the  $R = 0$  approximation in general does not satisfy the Fermi liquid condition. Therefore, the lowest order approximation is not applicable for the metallic state. Here we limit ourselves in the insulating state to demonstrate the quantitative aspect of the MLA within the lowest order approximation (RPT-0).

Calculated excitation spectra in the insulating regime are presented in Fig. 6. The result of the MLA is compared with the Hartree-Fock one and the NRG which is considered to be the best at zero temperature. The spectrum with use of the Hartree-Fock wavefunction indicates the insulator. But the upper and lower band widths are broader than those of the NRG. Static correlations localize the electrons and suppress such band broadening. Resulting spectrum in the MLA reproduces well the NRG one. The agreement of the spectra implies a quantitative description of the site-diagonal Green function according to the Lehmann representation of the

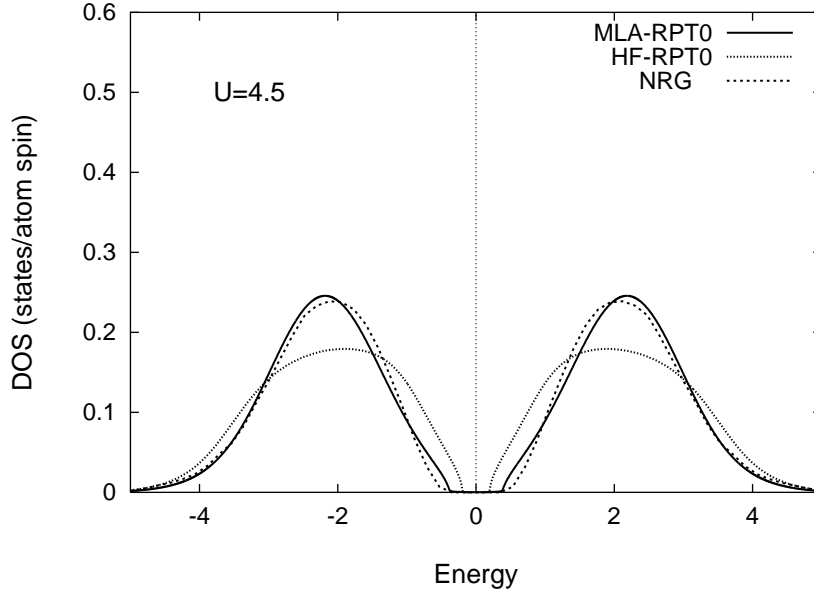


Fig. 6. Single-particle excitation spectra calculated by means of the RPT-0 plus MLA (MLA-RPT0: solid curve), the RPT-0 plus Hartree-Fock approximation (HF-RPT0: dotted curve),<sup>8</sup> and the numerical renormalization group method (NRG: dashed curve).<sup>20</sup>

Green function  $G^{(i)}(z)$ . In infinite dimensions, this means that the self-energy  $\tilde{\Sigma}(z)$  is described quantitatively by means of the present theory because of the CPA equation  $G^{(i)}(z) = F(z)$  and eq. (39).

The critical Coulomb interaction  $U_{c1}$  for gap formation is obtained from a condition that the insulator solution  $\text{Im}\tilde{\Sigma}(0^+) = -\infty$  disappears. This is equivalent to the following condition in the RPT-0 (see eq. (86) in Ref. 8).

$$U = 4\sqrt{c_2} . \quad (46)$$

Here  $c_2$  is the second moment of the memory function:  $c_2 = \int d\epsilon d\epsilon' d\epsilon'' \rho(\epsilon) \rho(\epsilon') \rho(\epsilon'') (\epsilon + \epsilon' - \epsilon'')^2 X(\epsilon, \epsilon', \epsilon'')$ .

For the wavefunction (10), the second moment  $c_2$  is given by the Hartree-Fock contribution  $c_2^{(0)} = 3/8 + 3\alpha^2/2$  and the correlation correction as

$$c_2 = c_2^{(0)} + \frac{c_2^{(2)}}{1 + \langle \tilde{O}_i^\dagger \tilde{O}_i \rangle_0} . \quad (47)$$

Here  $\alpha = 1/\sqrt{\pi}$  for the hypercubic lattice and  $\alpha = 4\sqrt{2}/3\pi$  for the Bethe lattice. The correlation contribution  $c_2^{(2)}$  in the second term at the r.h.s. of eq. (47) is given as follows.

$$c_2^{(2)} = 6 \int d\epsilon_1 d\epsilon_2 d\epsilon_3 \rho(\epsilon_1) \rho(\epsilon_2) \rho(\epsilon_3) (\epsilon_1 - \epsilon_2 - \epsilon_3)^2 [f(\epsilon_1) f(\epsilon_2) \kappa_1(-\epsilon_1 - \epsilon_2) - f(\epsilon_1) (1 - f(\epsilon_2)) \kappa_2(\epsilon_2, \epsilon_1) + f(\epsilon_1) (f(\epsilon_3) - f(\epsilon_2)) \lambda(-\epsilon_1)] , \quad (48)$$

Table I. Critical Coulomb interaction  $U_{c1}$  for the Bethe lattice in various approximations. MLA-RPT0: The MLA plus the lowest-order RPT in the PM-CPA (Present result), IPT: Iterative perturbation theory,<sup>22</sup> ED: Exact diagonalization method,<sup>23</sup> PSCT: Projective self-consistent technique,<sup>24</sup> LMA: Local moment approach,<sup>25</sup> NRG: Numerical renormalization group approach,<sup>20</sup>  $1/U$  Exp.:  $1/U$  expansion method.<sup>26</sup>

MLA-RPT0	IPT	ED	PSCT	LMA	NRG	$1/U$ Exp.
3.36	3.67	3.04	3.39	3.41	3.54	2.97

$$\kappa_1(\epsilon_k) = \int d\epsilon d\epsilon' \rho(\epsilon) \rho(\epsilon') f(\epsilon) (1 - f(\epsilon')) \kappa_0(\epsilon_k, \epsilon' - \epsilon) , \quad (49)$$

$$\kappa_2(\epsilon_k, \epsilon_{k'}) = \int d\epsilon d\epsilon' \rho(\epsilon) \rho(\epsilon') f(\epsilon) (1 - f(\epsilon')) \kappa_0(\epsilon_k - \epsilon, \epsilon' - \epsilon_{k'}) , \quad (50)$$

$$\lambda(\epsilon_k) = \int d\epsilon \rho(\epsilon) (1 - f(\epsilon)) \lambda_0(\epsilon_k, \epsilon) , \quad (51)$$

$$\kappa_0(\epsilon_k, \epsilon_{k'}) = \int d\epsilon d\epsilon' \rho(\epsilon) \rho(\epsilon') f(\epsilon) (1 - f(\epsilon')) \eta(\epsilon' - \epsilon + \epsilon_k) \eta(\epsilon' - \epsilon + \epsilon_{k'}) , \quad (52)$$

$$\begin{aligned} \lambda_0(\epsilon_k, \epsilon_{k'}) &= \int d\epsilon d\epsilon' d\epsilon'' \rho(\epsilon) \rho(\epsilon') \rho(\epsilon'') f(\epsilon) (1 - f(\epsilon')) f(\epsilon'') \\ &\quad \times \eta(\epsilon' - \epsilon - \epsilon'' + \epsilon_k) \eta(\epsilon' - \epsilon - \epsilon'' + \epsilon_{k'}) . \end{aligned} \quad (53)$$

Here  $\eta(\epsilon_k) \equiv U/(\epsilon_k - \epsilon_c)$ . See Appendix C for the actual expression of  $c_2^{(2)}$ .

We have determined the critical Coulomb interaction  $U_{c1}$  solving eq. (46). For a hypercubic lattice, we obtained  $U_{c1}(\text{MLA}) = 3.237$ , while we find  $U_{c1}(\text{HF}) = 3.693$  when we adopt the Hartree-Fock wave function. The reduction of  $U_{c1}$  due to electron correlations is understood from the DOS in Fig. 6. There we observe that the electron correlations on the static matrix elements enhance the Mott-Hubbard peaks at  $\omega = \pm U/2$ . It reduces the amplitude of DOS near the Fermi level, and therefore lowers the critical value  $U_{c1}$ .

The present value  $U_{c1}(\text{MLA}) = 3.237$  quantitatively agrees with the numerical result  $U_{c1}(\text{NRG}) = 3.25$  obtained by the NRG.<sup>20</sup> In the case of the Bethe lattice for which the noninteracting DOS is given by  $\rho(\epsilon) = \pi^{-1} \sqrt{2 - \epsilon^2}$ , we obtained  $U_{c1}(\text{MLA}) = 3.359$  and  $U_{c1}(\text{HF}) = 3.827$ . The critical value for the Bethe lattice has been calculated by various methods.<sup>20, 22-27</sup> These results are summarized in Table I together with the present result (MLA+RPT-0). There are some discrepancies in  $U_{c1}$  among the theories in case of the Bethe lattice. Our result agrees well with  $U_{c1} = 3.39$  obtained by the projective self-consistent technique (PSCT)<sup>24</sup> which is exact in the low energy region, and  $U_{c1} = 3.41$  obtained by the local moment approach (LMA).<sup>25</sup> Note that the results of the ED (Exact Diagonalization



Method)<sup>23</sup> and NRG<sup>20</sup> methods considerably depend on the way of line-broadening for the  $\delta$ -function spectrum in the case of the Bethe lattice. The present approach describes  $U_{c1}$  within 1% error for both the hypercubic and Bethe lattices.

The quantitative description of the excitation spectra for the Mott insulator with use of the RPT-0 may come as a surprise because the RPT is an approach starting from the weak Coulomb interaction limit due to the expansion of the screened memory function with respect to the interaction Liouvillean.<sup>8</sup> In this respect, it is worth pointing out that the RPT-0 can also describe the dynamics of the strongly correlated electrons via the effective medium and atomic self-energy in the denominator in eq. (41) since the RPT-0 memory function reduces to the Hubbard III approximation<sup>27</sup> in this region.

## 5. Summary

We have proposed a new local-ansatz wavefunction with momentum-dependent variational parameters (MLA) to improve the LA by Stollhoff and Fulde.<sup>6</sup> It is constructed by using the ‘flexible’ local operators which produce the two-particle excited states in the momentum space from the Hartree-Fock state and project those states onto the local excited states in the real space. The best wavefunction is chosen by controlling the momentum dependent variational parameters of the excited states in the momentum space on the basis of the variational principle. We obtained the ground-state energy of the MLA within a single-site approximation. Minimizing the energy, we derived a self-consistent equation for the variational parameters, and obtained an approximate solution which interpolates between the weak Coulomb interaction limit and the atomic limit. The correlation energy in the MLA agrees with the result of the second-order perturbation theory in infinite dimensions in the weak Coulomb interaction limit and yields the correct atomic limit as it should be.

We have investigated numerically the validity of the theory using the half-filled band Hubbard model in infinite dimensions. We verified that the MLA improves the LA in the whole range of the Coulomb interaction energy parameter  $U$ . For the hypercubic lattice, we found that the MLA yields the correlation energy lower than that of the GA in the range  $0 < U < 3.28$ . The double occupation number in the MLA is smaller than that of the LA irrespective of  $U$ . The GA overestimates the double occupancy in the range  $0 < U \lesssim 2$ , and underestimates it in the range  $U \gtrsim 3$ . We found that the MLA shows a reasonable energy dependence of the momentum distribution in the range  $0 < U \lesssim 3.0$ . This is qualitatively different from the LA and the GA because both of them lead to the energy-independent momentum distributions below and above the Fermi level. The quasiparticle weights in the MLA are very close to those of the NRG in the range  $0 < U \lesssim 2.5$ , while the LA and the GA overestimate them in general. These results suggest that the MLA is applicable to the systems with  $U/W \lesssim 1.5$ , for example, the systems like transition metals and alloys. Here  $W$  denotes the band width of the noninteracting system.

The critical Coulomb interaction  $U_{c2}$  in the MLA was obtained from the vanishment of the quasiparticle weights as  $U_{c2} = 3.21$ . It is comparable to  $U_{c2} = 4.10$  in the NRG, while the LA and the GA give larger values  $U_{c2} = 7.82$  and  $4.51$ , respectively.

We have also shown that the MLA combined with the PM-CPA is useful for understanding the correlation effects on the excitation spectra in the insulator regime. The MLA wavefunction allows us to calculate the static correlations in the retarded Green function obtained by the PM-CPA. We have demonstrated that the MLA+PM-CPA can quantitatively describe the excitation spectra in the insulator regime. Calculated critical Coulomb interactions  $U_{c1}$  for a gap formation agree with the best results obtained by the other methods within 1 % error for both the hypercubic and the Bethe lattices.

Although the present approach interpolates between the weak Coulomb interaction limit and the atomic limit, and much improves the LA, it does not describe the metal-insulator transition in a self-consistent way. The wavefunction continuously changes from the Hartree-Fock metallic state to the atomic one in the present theory, and does not show any anomaly at  $U_{c2}$  ( $U_{c1}$ ) obtained from the momentum distribution (the excitation spectra with use of the MLA+PM-CPA). Further improvements of the theory toward the strongly correlated region are desired to describe the metal-insulator transition in a self-consistent way.

## Acknowledgment

The authors would like to express our sincere thanks to Prof. P. Fulde for valuable discussions on our wavefunction.

## Appendix A: Average $\langle \tilde{A} \rangle$ in the single-site approximation

In this Appendix, we derive the formula (13) in the single-site approximation. Let us consider  $A_N$  and  $B_N$  such that

$$A_N = \left\langle \left[ \prod_i (1 - \tilde{O}_i^\dagger) \right] \tilde{A} \left[ \prod_i (1 - \tilde{O}_i) \right] \right\rangle_0, \quad (\text{A}\cdot 1)$$

$$B_N = \left\langle \left[ \prod_i (1 - \tilde{O}_i^\dagger) \right] \left[ \prod_i (1 - \tilde{O}_i) \right] \right\rangle_0. \quad (\text{A}\cdot 2)$$

Expanding  $B_N$  with respect to site 1, we obtain

$$\begin{aligned} B_N &= B_{N-1}^{(1)} - \left\langle \tilde{O}_1^\dagger \left[ \prod_i^{(1)} (1 - \tilde{O}_i^\dagger) \right] \left[ \prod_i^{(1)} (1 - \tilde{O}_i) \right] \right\rangle_0 \\ &\quad - \left\langle \left[ \prod_i^{(1)} (1 - \tilde{O}_i^\dagger) \right] \tilde{O}_1 \left[ \prod_i^{(1)} (1 - \tilde{O}_i) \right] \right\rangle_0 + \left\langle \tilde{O}_1^\dagger \left[ \prod_i^{(1)} (1 - \tilde{O}_i^\dagger) \right] \tilde{O}_1 \left[ \prod_i^{(1)} (1 - \tilde{O}_i) \right] \right\rangle_0, \end{aligned} \quad (\text{A}\cdot 3)$$

and

$$B_{N-1}^{(1)} = \left\langle \left[ \prod_i^{(1)} (1 - \tilde{O}_i^\dagger) \right] \left[ \prod_i^{(1)} (1 - \tilde{O}_i) \right] \right\rangle_0. \quad (\text{A}\cdot 4)$$

Here the product  $\prod_i^{(1)}$  means the product with respect to all the sites except site 1.

When we calculate  $B_N$  applying Wick's theorem, we neglect the contractions between different sites. This is a single-site approximation and then eq. (A.3) is expressed as

$$B_N = \langle (1 - \tilde{O}_1^\dagger)(1 - \tilde{O}_1) \rangle_0 B_{N-1}^{(1)}. \quad (\text{A.5})$$

We can make the same calculations for  $A_N$ . In this case, there are two-types of terms, the terms in which the operator  $\tilde{O}_1$  is contracted to  $\tilde{A}$  and the other terms with  $\tilde{O}_1$  contracted to the operators  $\tilde{O}_i$  ( $i \neq 1$ ). We have then

$$A_N = \langle (1 - \tilde{O}_1^\dagger)\tilde{A}(1 - \tilde{O}_1) \rangle_0 B_{N-1}^{(1)} + \langle (1 - \tilde{O}_1^\dagger)(1 - \tilde{O}_1) \rangle_0 A_{N-1}^{(1)}, \quad (\text{A.6})$$

and

$$A_{N-1}^{(1)} = \left\langle \left[ \prod_i^{(1)} (1 - \tilde{O}_i^\dagger) \right] \tilde{A} \left[ \prod_i^{(1)} (1 - \tilde{O}_i) \right] \right\rangle_0. \quad (\text{A.7})$$

Successive application of the recursive relations (A.5) and (A.6) leads to

$$A_N = \sum_i \langle (1 - \tilde{O}_i^\dagger)\tilde{A}(1 - \tilde{O}_i) \rangle_0 B_{N-1}^{(i)}, \quad (\text{A.8})$$

$$B_N = \langle (1 - \tilde{O}_1^\dagger)(1 - \tilde{O}_1) \rangle_0 B_{N-1}^{(1)} = \prod_i \langle (1 - \tilde{O}_i^\dagger)(1 - \tilde{O}_i) \rangle_0. \quad (\text{A.9})$$

Taking the ratio  $A_N/B_N$ , we reach eq. (13).

$$\langle \tilde{A} \rangle = \sum_i \frac{\langle (1 - \tilde{O}_i^\dagger)\tilde{A}(1 - \tilde{O}_i) \rangle_0}{\langle (1 - \tilde{O}_i^\dagger)(1 - \tilde{O}_i) \rangle_0}. \quad (\text{A.10})$$

## Appendix B: Laplace transform for the correlation calculations

Using the relation

$$\frac{1}{z - \epsilon_4 + \epsilon_3 - \epsilon_2 + \epsilon_1 + \epsilon_c} = -i \int_0^\infty dt e^{i(z - \epsilon_4 + \epsilon_3 - \epsilon_2 + \epsilon_1 + \epsilon_c)t}, \quad (\text{B.1})$$

we can reduce the number of integrals in the physical quantities. Here  $z = \omega + i\delta$ , and  $\delta$  is an infinitesimal positive number. Laplace transforms of various elements in the physical quantities are summarized as follows.

$$\begin{aligned} \langle \tilde{H}\tilde{O}_i \rangle_0 &= \langle \tilde{O}_i^\dagger \tilde{H} \rangle_0^* \\ &= iU^2 [1 - \eta(1 - 2\langle n_{i\uparrow} \rangle_0)(1 - 2\langle n_{i\downarrow} \rangle_0)] \int_0^\infty dt e^{i\epsilon_c t} a_\uparrow(-t) a_\downarrow(-t) b_\uparrow(t) b_\downarrow(t). \quad (\text{B.2}) \\ \langle \tilde{O}_i^\dagger \tilde{H} \tilde{O}_i \rangle_0 &= -U^2 [1 - \eta(1 - 2\langle n_{i\uparrow} \rangle_0)(1 - 2\langle n_{i\downarrow} \rangle_0)]^2 \\ &\quad \times \int_0^\infty dt dt' e^{i\epsilon_c(t+t')} [a_\uparrow(-t-t') b_\uparrow(t+t') a_\downarrow(-t-t') b_{1\downarrow}(t+t') \\ &\quad - a_\uparrow(-t-t') b_\uparrow(t+t') a_{1\downarrow}(-t-t') b_\downarrow(t+t') \\ &\quad + a_\uparrow(-t-t') b_{1\uparrow}(t+t') a_\downarrow(-t-t') b_\downarrow(t+t') \end{aligned}$$

$$-a_{1\uparrow}(-t-t')b_{\uparrow}(t+t')a_{\downarrow}(-t-t')b_{\downarrow}(t+t')], \quad (\text{B}\cdot 3)$$

$$\begin{aligned} \langle \tilde{O}_i^\dagger O_i \tilde{O}_i \rangle_0 &= -U^2 [1 - \eta(1 - 2\langle n_{i\uparrow} \rangle_0)(1 - 2\langle n_{i\downarrow} \rangle_0)]^2 \\ &\times \int_0^\infty dt dt' e^{i\epsilon_c(t+t')} [a_{\uparrow}(-t)b_{\uparrow}(t+t')a_{\downarrow}(-t)b_{\downarrow}(t+t')a_{\uparrow}(-t')a_{\downarrow}(-t') \\ &\quad - a_{\uparrow}(-t)b_{\uparrow}(t+t')a_{\downarrow}(-t-t')b_{\downarrow}(t)a_{\uparrow}(-t')b_{\downarrow}(t') \\ &\quad - a_{\uparrow}(-t-t')b_{\uparrow}(t)a_{\downarrow}(-t)b_{\downarrow}(t+t')b_{\uparrow}(t')a_{\downarrow}(-t') \\ &\quad + a_{\uparrow}(-t-t')b_{\uparrow}(t)a_{\downarrow}(-t-t')b_{\downarrow}(t)b_{\uparrow}(t')b_{\downarrow}(t')] , \quad (\text{B}\cdot 4) \end{aligned}$$

$$\begin{aligned} \langle \tilde{O}_i^\dagger \tilde{O}_i \rangle_0 &= -U^2 [1 - \eta(1 - 2\langle n_{i\uparrow} \rangle_0)(1 - 2\langle n_{i\downarrow} \rangle_0)]^2 \\ &\times \int_0^\infty dt dt' e^{i\epsilon_c(t+t')} a_{\uparrow}(-t-t')b_{\uparrow}(t+t')a_{\downarrow}(-t-t')b_{\downarrow}(t+t') . \quad (\text{B}\cdot 5) \end{aligned}$$

Here

$$a_{\sigma}(t) = \int d\epsilon \rho(\epsilon) f(\epsilon + \tilde{\epsilon}_{\sigma}) e^{-i\epsilon t} , \quad (\text{B}\cdot 6)$$

$$b_{\sigma}(t) = \int d\epsilon \rho(\epsilon) (1 - f(\epsilon + \tilde{\epsilon}_{\sigma})) e^{-i\epsilon t} , \quad (\text{B}\cdot 7)$$

$$a_{1\sigma}(t) = \int d\epsilon \rho(\epsilon) f(\epsilon + \tilde{\epsilon}_{\sigma}) \epsilon e^{-i\epsilon t} , \quad (\text{B}\cdot 8)$$

$$b_{1\sigma}(t) = \int d\epsilon \rho(\epsilon) (1 - f(\epsilon + \tilde{\epsilon}_{\sigma})) \epsilon e^{-i\epsilon t} , \quad (\text{B}\cdot 9)$$

and  $\tilde{\epsilon}_{\sigma} = \epsilon_0 + U\langle n_{i-\sigma} \rangle_0 - \mu$  is the Hartree-Fock level measured from the Fermi level  $\mu$ .  $\rho(\epsilon)$  in the above expressions denotes the density of states for  $\epsilon_k$ , *i.e.*, the Fourier transform of  $t_{ij}$ .

Correlation contribution to the momentum distribution function (36) is given by

$$\begin{aligned} N\langle \tilde{O}_i^\dagger \tilde{n}_{k\sigma} \tilde{O}_i \rangle_0 &= -2U^2 [1 - \eta(1 - 2\langle n_{i\uparrow} \rangle_0)(1 - 2\langle n_{i\downarrow} \rangle_0)]^2 \\ &\times \int_0^\infty dt dt' e^{i\epsilon_c(t+t')} a_{\sigma}(t+t')b_{\sigma}(-t-t') \\ &\times [f(\epsilon_{k\sigma})a_{-\sigma}(t+t')e^{-i\epsilon_c(t+t')} - (1 - f(\epsilon_{k\sigma}))a_{-\sigma}(-t-t')e^{i\epsilon_c(t+t')}] . \quad (\text{B}\cdot 10) \end{aligned}$$

Correlation contribution to the electron number (35) which appears in the calculation of the double occupation number is expressed as

$$\begin{aligned} \langle \tilde{O}_i^\dagger \tilde{n}_{i\sigma} \tilde{O}_i \rangle_0 &= -U^2 [1 - \eta(1 - 2\langle n_{i\uparrow} \rangle_0)(1 - 2\langle n_{i\downarrow} \rangle_0)]^2 \\ &\times \int_0^\infty dt dt' e^{i\epsilon_c(t+t')} [a_{-\sigma}(-t-t')b_{-\sigma}(t+t')a_{\sigma}(-t-t')b_{\sigma}(t)b_{\sigma}(t') \\ &\quad - a_{-\sigma}(-t-t')b_{-\sigma}(t+t')a_{\sigma}(-t)b_{\sigma}(t+t')a_{\sigma}(t')] . \quad (\text{B}\cdot 11) \end{aligned}$$

The element (37) for the calculation of the double occupancy is expressed as

$$\langle \tilde{O}_i^\dagger O_i \rangle_0 + \langle O_i \tilde{O}_i \rangle_0 = -2iU [1 - \eta(1 - 2\langle n_{i\uparrow} \rangle_0)(1 - 2\langle n_{i\downarrow} \rangle_0)]$$

$$\times \int_0^\infty dt e^{i\epsilon_c t} a_\uparrow(-t) b_\uparrow(t) a_\downarrow(-t) b_\downarrow(t) . \quad (\text{B}\cdot 12)$$

### Appendix C: Expressions of $X(\epsilon, \epsilon', \epsilon'')$ , $\bar{G}_{0\sigma}^{(i)}(z)$ , and $c_2^{(2)}$ in the MLA

In the  $R = 0$  approximation, the correlation function  $X(\epsilon, \epsilon', \epsilon'')$  given by eq. (44) is obtained from the formula (13) as

$$X(\epsilon, \epsilon', \epsilon'') = \chi(\epsilon, \epsilon', \epsilon'') - \frac{X_1(\epsilon, \epsilon', \epsilon'')}{1 + \langle \tilde{O}_i^\dagger \tilde{O}_i \rangle_0} + \frac{X_2(\epsilon, \epsilon', \epsilon'')}{1 + \langle \tilde{O}_i^\dagger \tilde{O}_i \rangle_0} . \quad (\text{C}\cdot 1)$$

For the half-filled band, we have

$$\chi(\epsilon, \epsilon', \epsilon'') = f(-\epsilon)f(-\epsilon')f(\epsilon'') + f(\epsilon)f(\epsilon')f(-\epsilon'') , \quad (\text{C}\cdot 2)$$

$$\begin{aligned} X_1(\epsilon, \epsilon', \epsilon'') &= -f(\epsilon'')f(-\epsilon)\nu(\epsilon - \epsilon'') - f(-\epsilon'')f(\epsilon)\nu(\epsilon'' - \epsilon) \\ &\quad + f(-\epsilon')f(-\epsilon)\nu(\epsilon + \epsilon') + f(\epsilon')f(\epsilon)\nu(-\epsilon - \epsilon') , \end{aligned} \quad (\text{C}\cdot 3)$$

$$\begin{aligned} X_2(\epsilon, \epsilon', \epsilon'') &= f(-\epsilon')f(\epsilon'')\kappa_1(\epsilon' - \epsilon'') - f(\epsilon')f(\epsilon'')\kappa_2(-\epsilon', \epsilon'') \\ &\quad - f(-\epsilon')f(-\epsilon'')\kappa_2(\epsilon', -\epsilon'') + f(\epsilon')f(-\epsilon'')\kappa_1(\epsilon'' - \epsilon') \\ &\quad - f(\epsilon'')f(\epsilon)\kappa_2(-\epsilon'', \epsilon) + f(\epsilon'')f(-\epsilon)\kappa_1(\epsilon - \epsilon'') \\ &\quad + f(-\epsilon'')f(\epsilon)\kappa_1(\epsilon'' - \epsilon) - f(-\epsilon'')f(-\epsilon)\kappa_2(\epsilon'', -\epsilon) \\ &\quad + f(\epsilon')f(\epsilon)\kappa_1(-\epsilon' - \epsilon) - f(\epsilon')f(-\epsilon)\kappa_2(\epsilon, \epsilon') \\ &\quad - f(-\epsilon')f(\epsilon)\kappa_2(\epsilon', \epsilon) + f(-\epsilon')f(-\epsilon)\kappa_1(\epsilon' + \epsilon) \\ &\quad + (f(\epsilon) - f(\epsilon''))[f(-\epsilon')\lambda(\epsilon') - f(\epsilon')\lambda(-\epsilon')] \\ &\quad - (f(-\epsilon) - f(\epsilon'))[f(\epsilon'')\lambda(-\epsilon'') - f(-\epsilon'')\lambda(\epsilon'')] \\ &\quad + (f(\epsilon'') - f(\epsilon'))[f(\epsilon)\lambda(-\epsilon) - f(-\epsilon)\lambda(\epsilon)] . \end{aligned} \quad (\text{C}\cdot 4)$$

Here  $\nu(\epsilon)$  is defined by

$$\nu(\epsilon_k) = \int d\epsilon d\epsilon' \rho(\epsilon)\rho(\epsilon')f(\epsilon)f(-\epsilon')\eta(\epsilon' - \epsilon + \epsilon_k) , \quad (\text{C}\cdot 5)$$

$\eta(\epsilon)$  is defined by  $\eta(\epsilon) = U/(\epsilon - \epsilon_c)$ .  $\kappa_1(\epsilon)$ ,  $\kappa_2(\epsilon, \epsilon')$ , and  $\lambda(\epsilon)$  in  $X_2$  are defined by eqs. (49), (50), and (51), respectively.

Substituting eq. (C·1) into eq. (43) and making use of the Laplace transform (B·1), we obtain the expression for  $\bar{G}_{0\sigma}^{(i)}(z)$  with use of the Laplace transform as

$$\bar{G}_{0\sigma}^{(i)}(z) = M_0(z - \tilde{\Sigma}(z)) + \frac{M_2(z - \tilde{\Sigma}(z))}{1 + \langle \tilde{O}_i^\dagger \tilde{O}_i \rangle_0} , \quad (\text{C}\cdot 6)$$

$$M_0(z) = -i \int dt e^{izt} (b(-t)^3 + b(t)^3) , \quad (\text{C}\cdot 7)$$

$$M_2(z) = -3i \int dt e^{izt} \phi(t) [\kappa_1(t) - \kappa_2(t) + (b(-t) - b(t))\lambda_1(t)] , \quad (\text{C}\cdot 8)$$

$$\kappa_1(t) = -U^2 \int dt' dt'' e^{i\epsilon_c(t'+t'')} (b(t+t')^2 + b(t'-t)^2) b(t'+t'')^2 b(t'')^2 , \quad (\text{C}\cdot 9)$$

$$\kappa_2(t) = -2U^2 \int dt' dt'' e^{i\epsilon_c(t'+t'')} b(t') b(t+t') b(t'') b(t''-t) b(t'+t'')^2 , \quad (\text{C}\cdot 10)$$

$$\lambda_1(t) = -U^2 \int dt' dt'' e^{i\epsilon_c(t'+t'')} (b(t+t') - b(t'-t)) b(t'+t'')^3 b(t'') . \quad (\text{C}\cdot 11)$$

Here  $\phi(t) = \int d\epsilon \rho(\epsilon) e^{i\epsilon t}$ , and we used the relation  $a(t) = b(-t)$  for the half-filled and symmetric band.

In the same way, the correlation contribution  $c_2^{(2)}$  to the second moment of the memory function (*i.e.*, eq. (48)) is expressed as

$$c_2^{(2)} = -12U^2 \int dt dt' e^{i\epsilon_c(t+t')} b(t+t')^2 b_1(t) b(t') [b_1(t) b(t') + b(t) b_1(t') - \alpha b(t+t')] . \quad (\text{C}\cdot 12)$$

Here  $\alpha = 1/\sqrt{\pi}$  for the hypercubic lattice and  $\alpha = 4\sqrt{2}/3\pi$  for the Bethe lattice.  $b(t)$  and  $b_1(t)$  are defined by eqs. (B.7) and (B.9), respectively.

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